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5-Chloro-2-nitroaniline

Seik Weng Ng

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.122
Data-to-parameter ratio = 13.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_6H_5ClN_2O_2$, exists as a planar molecule; adjacent molecules are linked by N···O hydrogen bonds into ribbons.

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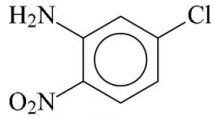
Comment

Chloronitroanilines possess non-linear optical properties. The crystal structure of 5-chloro-2-aniline, (I), was presented at a conference (Gerbi *et al.*, 1988), but it has not been abstracted into the Cambridge Structural Database (Version 5.26; Allen, 2002). The first chloronitroaniline to be authenticated was 2-chloro-4-nitroaniline (McPhail & Sim, 1965); chloronitroanilines are generally not well studied, and 4,5-dichloro-2-nitroaniline (Doyle, 1999) represents a rare example. The title compound (Fig. 1) exists as a planar molecule; adjacent molecules are linked by hydrogen bonds (Table 1) into a ribbon (Fig. 2).



(I)

Experimental

The title compound was obtained commercially and was recrystallized from dimethyl sulfoxide.

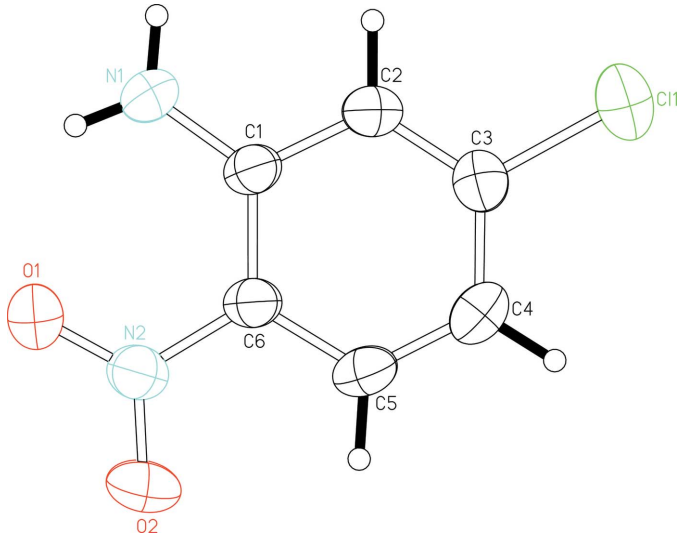


Figure 1
ORTEPII plot (Johnson, 1976) of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

Crystal data

$C_6H_5ClN_2O_2$
$M_r = 172.57$
Triclinic, $P\overline{1}$
$a = 7.073$ (3) Å
$b = 7.423$ (3) Å
$c = 7.711$ (3) Å
$\alpha = 83.87$ (3)°
$\beta = 81.98$ (3)°
$\gamma = 62.24$ (3)°
$V = 354.4$ (3) Å^3
$Z = 2$
$D_x = 1.617$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3038 reflections
$\theta = 3.1$–27.5°
$\mu = 0.48$ mm^{-1}
$T = 295$ (2) K
Plate, yellow
0.32 × 0.21 × 0.01 mm

Data collection

Rigaki R-AXIS RAPID IP diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.505$, $T_{max} = 0.955$
3525 measured reflections
1608 independent reflections
1299 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 27.5$°
$h = -9 \rightarrow 9$
$k = -7 \rightarrow 9$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.122$
$S = 1.07$
1608 reflections
120 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0843P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H11···O1	0.84 (1)	2.07 (2)	2.633 (2)	124 (2)
N1—H11···O1^{i}	0.84 (1)	2.45 (2)	3.152 (2)	141 (2)
N1—H12···O2^{ii}	0.85 (1)	2.35 (1)	3.113 (2)	150 (2)

Symmetry codes: (i) $-x+1, -y, -z+2$; (ii) $x+1, y, z$.

H atoms were located in difference Fourier maps and were refined with distance restraints of N—H = 0.85 (1) Å and C—H = 0.95 (1) Å.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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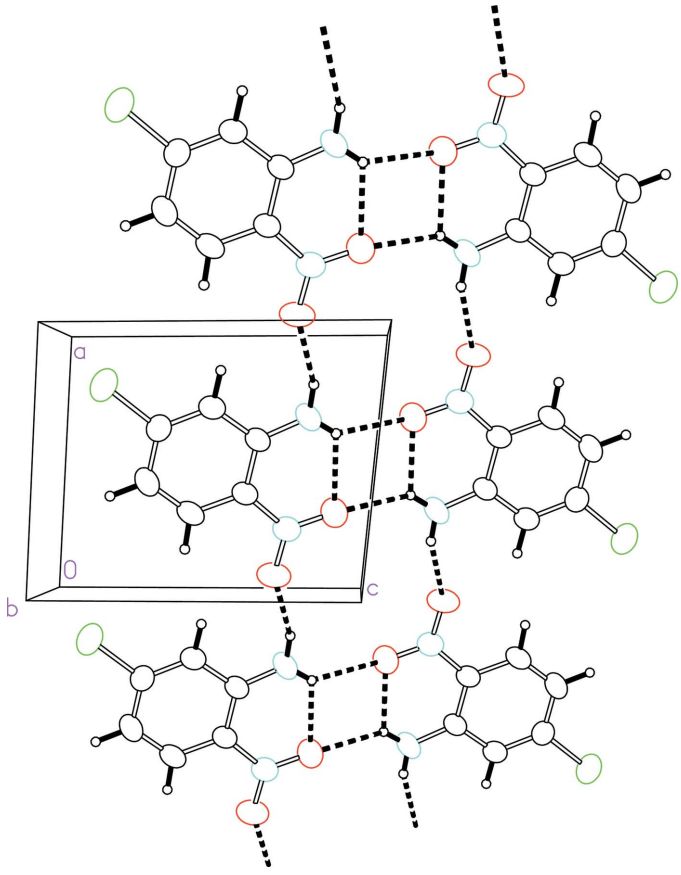

Figure 2
ORTEPII plot (Johnson, 1976) of the ribbon structure of (I). Dashed lines indicate hydrogen bonds.

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